

# Tailoring Frustrated Lewis Pair Catalysts for Enhanced Electrochemical CO<sub>2</sub> Reduction to Multi-Carbon Fuels

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## Computational methods

The calculations in this work were performed using spin-polarized density functional theory (DFT) as implemented in the Vienna Ab-initio Simulation Package (VASP).<sup>1,2</sup> The electron-ion interactions were described by the projector augmented wave (PAW) method<sup>3</sup> and The Perdew-Burke-Ernzerhof (PBE) functional was used as an exchange-correlation functional approximation.<sup>4,5</sup> The van der Waals (vdW) correction proposed by Grimme (DFT-D2) was employed to describe long-range vdW interactions.<sup>6</sup> The crystal structures of boron phosphide (BP) and boron arsenide (BAs) are modeled based on their bulk properties. Lattice constants are  $a=b=c=4.55\text{ \AA}$  and  $a=b=c=4.77\text{ \AA}$ . Both materials adopt a cubic structure, which belongs to the space group F-43m. The BP/BAs (110) surfaces were modeled with  $3\times 2$  supercells, and six atomic layers were used. During structure optimization, the adsorbates and the 4 topmost layers were allowed to relax in all directions while the 2 bottom layers were fixed at the optimized bulk positions (See Fig. S10). A plane wave basis set with an energy cutoff of 450 eV was used. In geometry optimizations, all the atomic coordinates were fully relaxed up to the residual atomic forces smaller than  $0.02\text{ eV/\AA}$ , and the total energy was converged to  $10^{-4}\text{ eV}$ . The vertical separation between periodic slabs was more than  $16\text{ \AA}$  in all cases. The Brillouin zones of all surfaces were sampled with  $5\times 5\times 1$  Monkhorst-Pack grids. The climbing-image nudged elastic band (CI-NEB) method<sup>7</sup> was employed to locate the minimum energy paths. All intermediate images of each CI-NEB simulation were relaxed until the forces converged to  $0.05\text{ eV/\AA}$ . Ab initio molecular dynamics (AIMD) simulations were performed in the canonical ensemble with a time step of 1.0 fs. The temperature was set to 500 K using the Nose-Hoover method.<sup>8</sup> The AIMD simulations of the BP and BAs (110) surfaces in an aqueous electrolyte environment containing alkali metal ions ( $\text{Na}^+$ ) and 30 explicit water molecules.

The free energy changes at each electrochemical step involving a proton-electron transfer were computed based on computational hydrogen electrode (CHE) model<sup>9,10</sup>, in which the free energy of ( $\text{H}^+ + \text{e}^-$ ) equals to  $1/2\text{H}_2(\text{g})$  for standard hydrogen electrode (SHE). The free energy of adsorbates and non-adsorbed gas-phase molecules is calculated as  $G = E_{\text{DFT}} + E_{\text{ZPE}} + \int C_p dT - TS$ , where  $E_{\text{DFT}}$  is the electronic energy calculated by DFT,  $E_{\text{ZPE}}$  is the zero-point energy (ZPE),  $C_p$  is heat capacity,  $T$  and  $S$  is temperature and entropy, respectively.

**Calculation methods of free energy difference:**

$$\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S + \int C_p dT$$

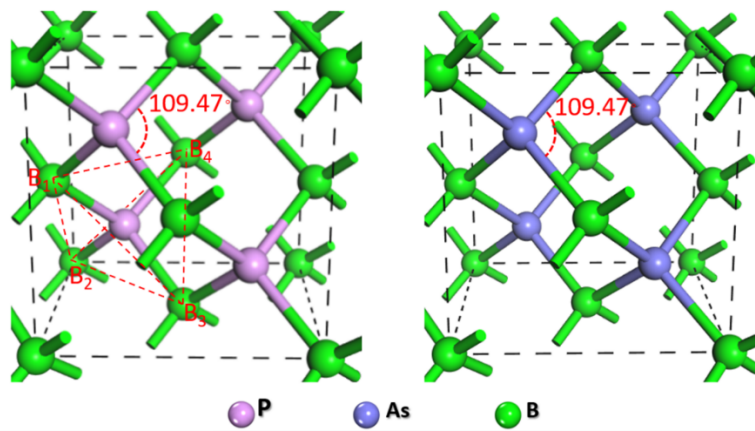
The  $\Delta E_{ZPE}$ ,  $T\Delta S$  and  $\int C_p dT$  for each reaction intermediates can be calculated by the following equations, respectively:

$$E_{ZPE} = \frac{1}{2} \sum_i h\nu_i$$

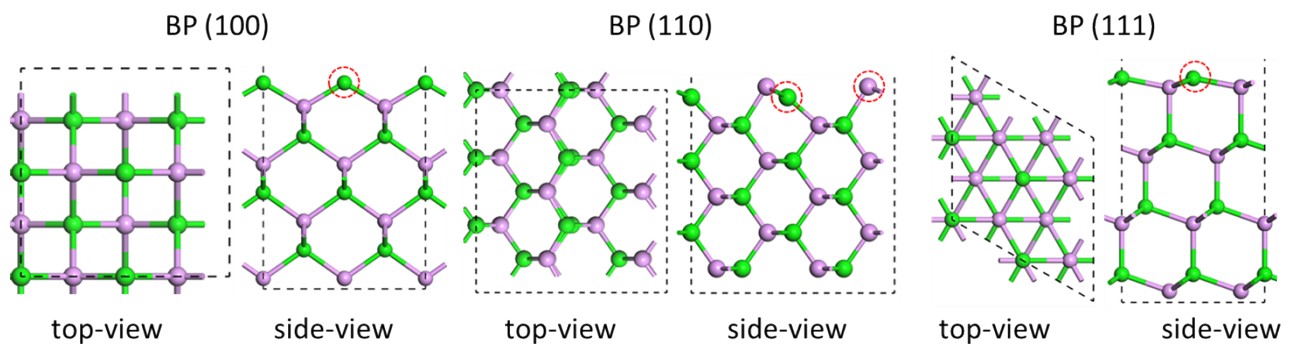
$$-TS = k_B T \sum_i \ln \left( 1 - e^{-\frac{h\nu_i}{k_B T}} \right) - \sum_i h\nu_i \left( \frac{1}{e^{\frac{h\nu_i}{k_B T}} - 1} \right)$$

$$\int C_p dT = \sum_i h\nu_i \left( \frac{1}{e^{\frac{h\nu_i}{k_B T}} - 1} \right)$$

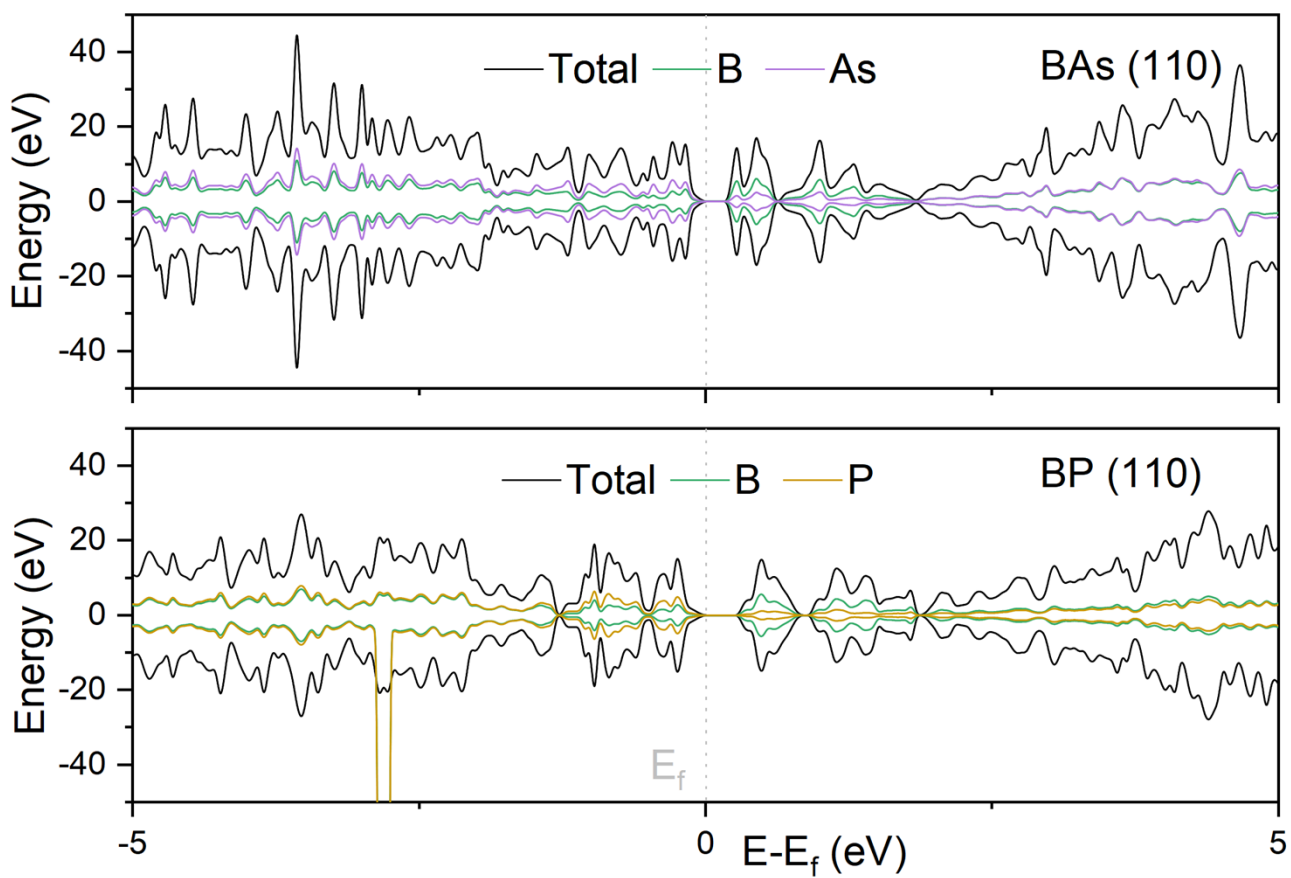
In the equations above,  $h$ ,  $\nu$  and  $k_B$  are Planck constant, vibrational frequencies, and Boltzmann constant, respectively. Besides, only when we calculate the free energy of reaction intermediates, the zero-point energy, entropy, and enthalpy are needed to calculate.



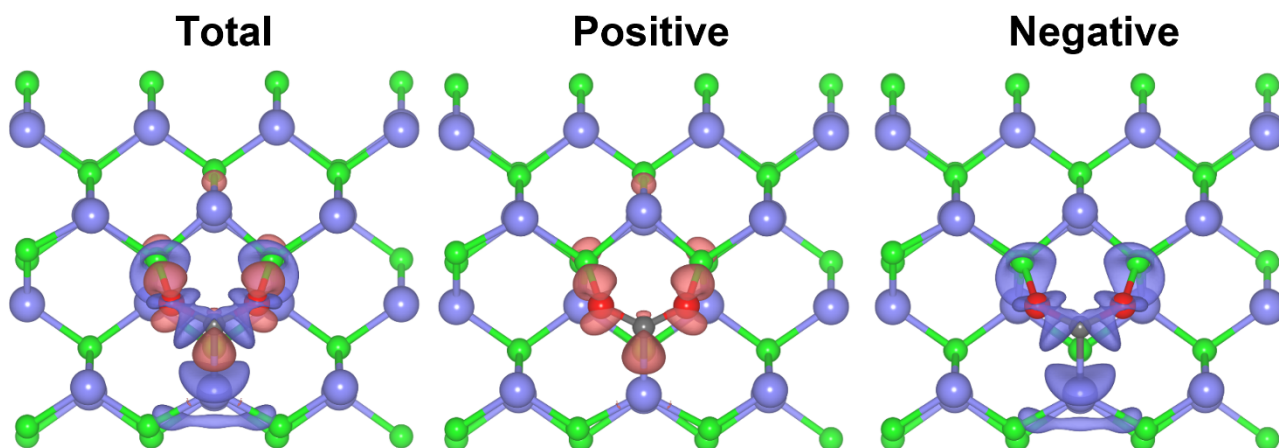
**Fig. S1** The structure of BP and BA5 unit-cell. The cubic BP and BA5 present a typical  $sp^3$  hybridization with a tetrahedral configuration and a bond angle of  $109.47^\circ$ .



**Fig. S2** Schematic atomic structures of (a) the (100) surface, (b) the (110) surface, and (c) the (111) surface of cubic BP. The red circles represent the exposed sites with surface dangling bonds.

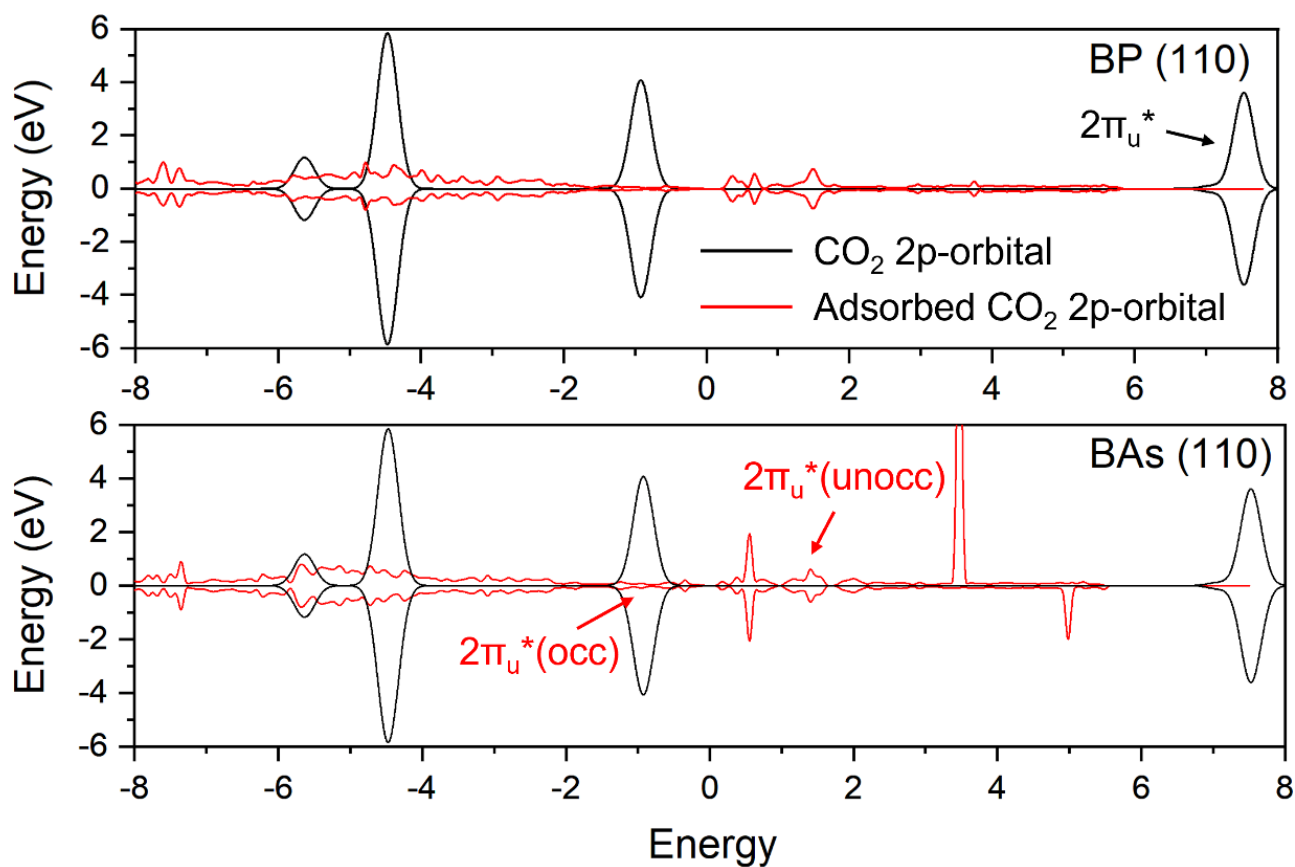


**Fig. S3** The PDOS of BAs and BP (110) surface. A high density of states near the conduction band minimum and the valence band maximum, which suggests that the carrier mobility should be quite favorable in these regions despite the semiconducting nature.

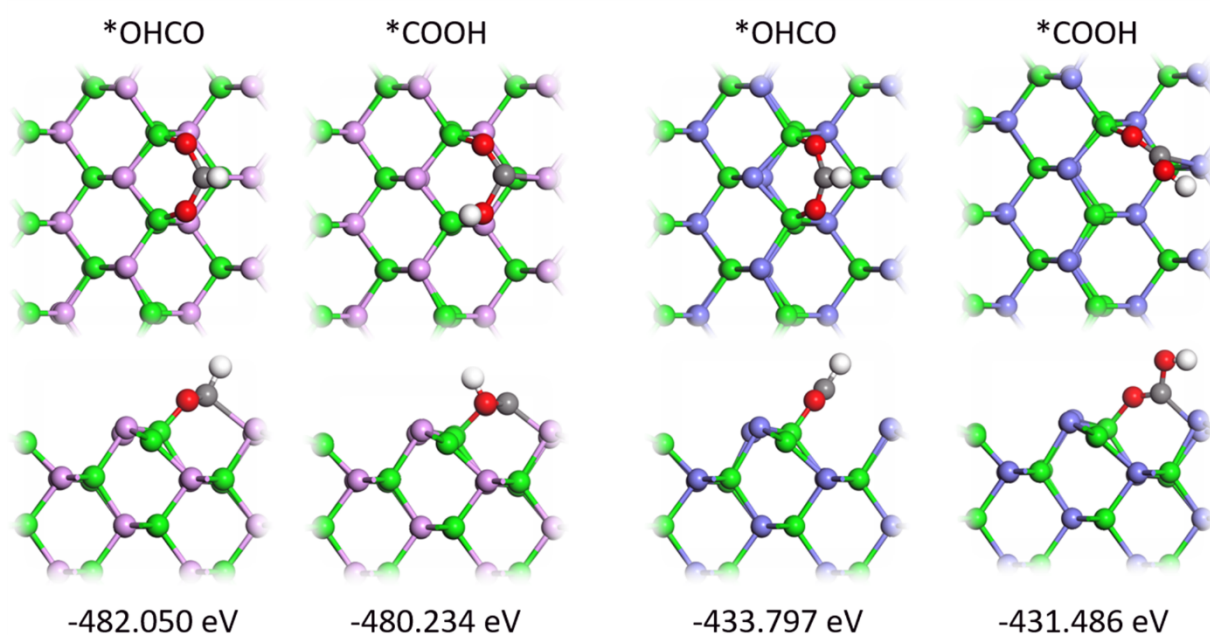


**Fig. S4** Configuration and charge density difference for CO<sub>2</sub> molecule adsorbed on BAs (110)

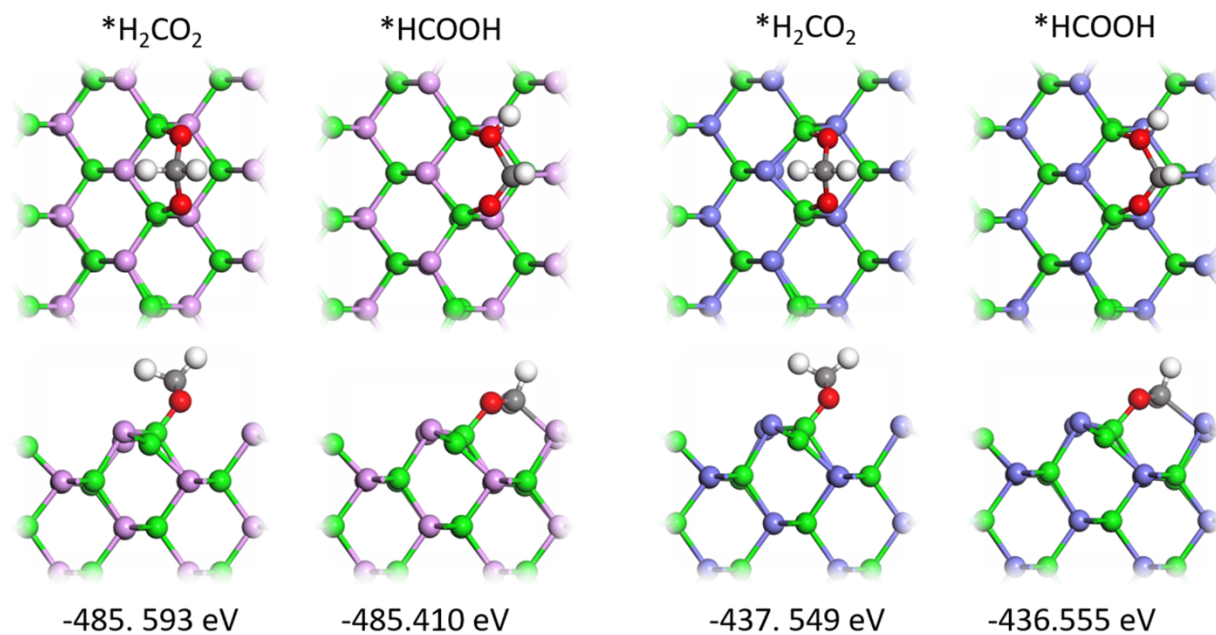
surface and the isosurface value is set at  $8.5 \times 10^{-4} \text{ e/Bohr}^3$ . Red represents electron accumulation and blue refers to electron depletion.



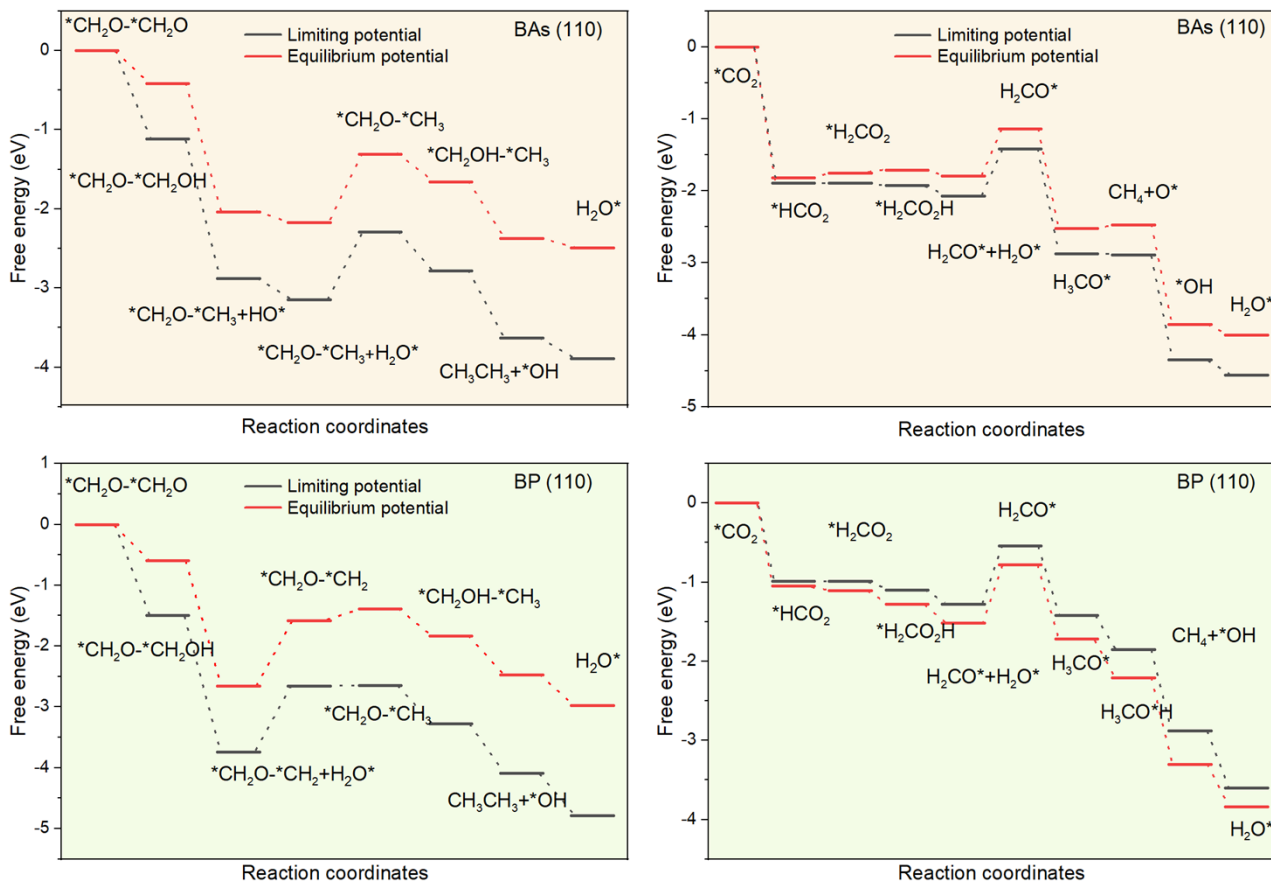
**Fig. S5** The PDOS of the isolated CO<sub>2</sub> molecule and the CO<sub>2</sub> adsorbed on BAs and BP (110) surface.



**Fig. S6** Structures (top and side views) of \*OCHO and \*COOH adsorbed on BP and BAs (110) surface.

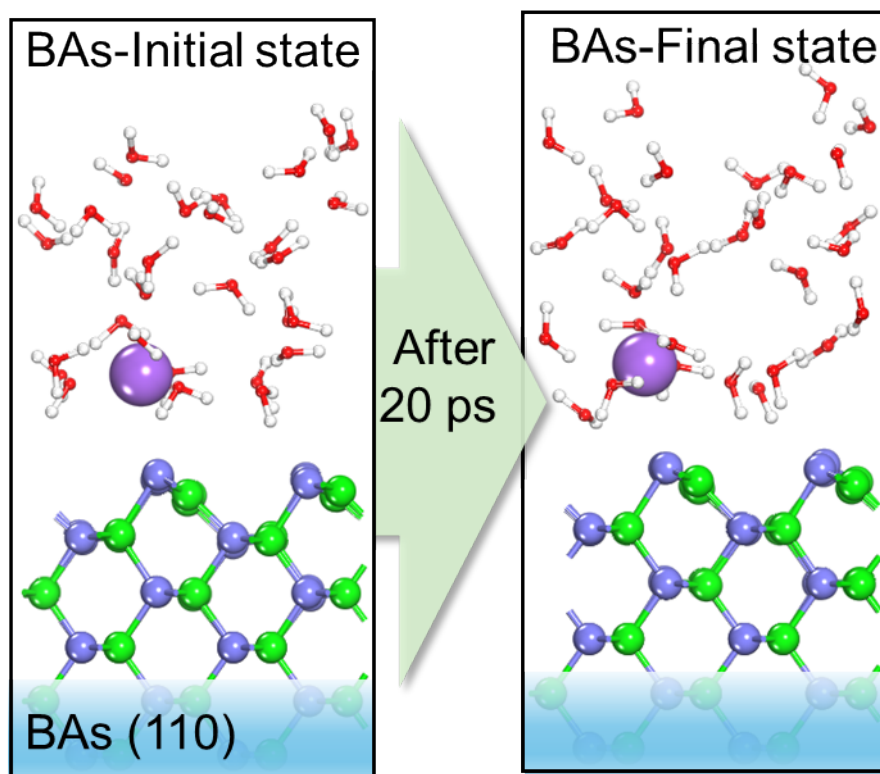


**Fig. S7** Structures (top and side views) of \*H<sub>2</sub>CO<sub>2</sub> and \*HCOOH adsorbed on BP and BAs (110) surface.



**Fig. S8** Free energy diagrams for CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> formation from the initial CO<sub>2</sub> activation at equilibrium and limiting potential conditions.





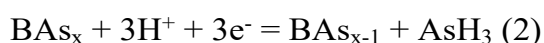
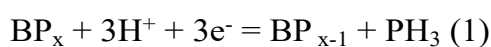
**Fig. S9** AIMD simulations of BAS (110) under electrochemical conditions. Oxygen, hydrogen, boron, arsenic, and Na atoms are red, white, light green, dark blue, and dark purple, respectively.

**Table S1** The dissolution potential of P and As for BP and BAs (110) surface, respectively.

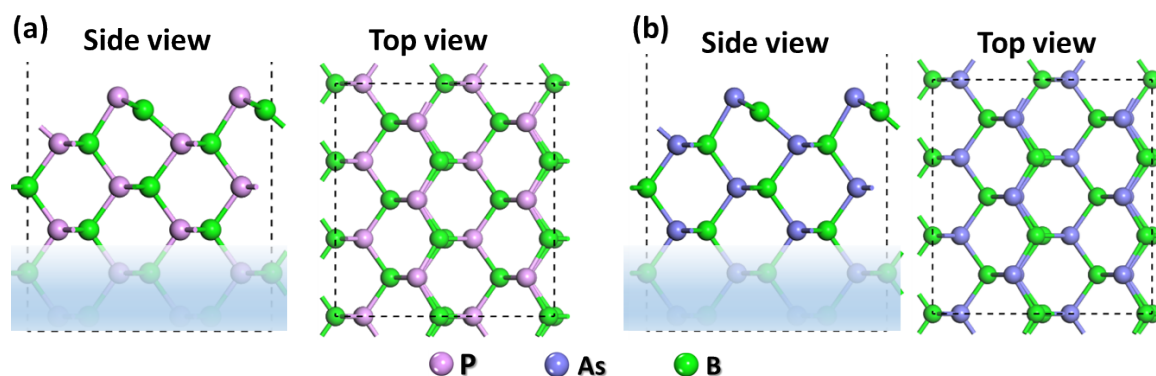
Dissolution process	dissolution potential (V)
P dissolution	-4.43
As dissolution	-3.65

The dissolution potentials of surface P and As atoms is simply estimated by DFT calculations.

The dissolution process can be described by the following chemical reactions:



In these reactions, surface P and As atoms are reduced to  $\text{PH}_3$  and  $\text{AsH}_3$ , respectively, through proton-coupled electron transfer. The dissolution potential ( $U_{\text{diss}}$ ) is defined as:  $U_{\text{diss}} = -\Delta G/e$ . Our calculations show that the dissolution potentials for both P and As are very high, as summarized in Table S1. This indicates that a significant potential is required for the electrodisolution of P and As, suggesting that the materials are thermodynamically stable under the reaction conditions.



**Fig. S10** Schematic atomic structures of (a) the (110) surface of cubic BP and (b) the (110) surface of cubic BAs. The layers inside the blue rectangle regions are fixed to bulk positions while other layers are relaxed.

### The coordinates files of CH<sub>4</sub> formation on BP (110)

\*CO<sub>2</sub>

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	C	O	P
36	1	2	36

Direct

0.000000000	0.000000000	0.069811001
0.002446000	0.000024000	0.209822997
0.977783024	0.000077000	0.332183987
0.250000000	0.166666999	0.000000000
0.256224006	0.168479994	0.281255990
0.250000000	0.166666999	0.139621004
0.500000000	0.000000000	0.069811001
0.499491006	0.000022000	0.209047005
0.474783003	0.000044000	0.335664004
0.750000000	0.166666999	0.000000000
0.747555971	0.167976007	0.277776003
0.750000000	0.166666999	0.139621004
0.000000000	0.333332986	0.069811001
0.000146000	0.332040995	0.208663002
0.973336995	0.326002002	0.334322989
0.250000000	0.500000000	0.000000000
0.249109998	0.500051022	0.277976990
0.250000000	0.500000000	0.139621004
0.500000000	0.333332986	0.069811001
0.498120993	0.333337009	0.207649007
0.498084992	0.343093991	0.344606996

0.750000000	0.500000000	0.000000000
0.744427025	0.500042975	0.273299992
0.750000000	0.500000000	0.139621004
0.000000000	0.666666985	0.069811001
0.000149000	0.668011010	0.208663002
0.973322988	0.674161017	0.334327996
0.250000000	0.833333015	0.000000000
0.256231010	0.831613004	0.281262010
0.250000000	0.833333015	0.139621004
0.500000000	0.666666985	0.069811001
0.498126000	0.666712999	0.207651004
0.498077005	0.657005012	0.344612986
0.750000000	0.833333015	0.000000000
0.747559011	0.832102001	0.277776986
0.750000000	0.833333015	0.139621004
0.692905009	0.500042975	0.386664003
0.629674971	0.619504988	0.389773995
0.629689991	0.380611002	0.389762998
0.125000000	0.000000000	0.000000000
0.125000000	0.000000000	0.139621004
0.136153996	0.000043000	0.279877990
0.375483990	0.167044997	0.209307000
0.375000000	0.166666999	0.069811001
0.377797991	0.170710996	0.355569005
0.625000000	0.000000000	0.000000000
0.625000000	0.000000000	0.139621004
0.627574027	0.000036000	0.279159993
0.876465976	0.166007996	0.209166005
0.875000000	0.166666999	0.069811001
0.868314981	0.162634999	0.353399009

0.125000000	0.333332986	0.000000000
0.125000000	0.333332986	0.139621004
0.128555000	0.333292007	0.278798997
0.374431014	0.500027001	0.208472997
0.375000000	0.500000000	0.069811001
0.361600995	0.500045002	0.349969000
0.625000000	0.333332986	0.000000000
0.625000000	0.333332986	0.139621004
0.622344017	0.332635999	0.275748998
0.878584027	0.500028014	0.207678005
0.875000000	0.500000000	0.069811001
0.872482002	0.500073016	0.345789999
0.125000000	0.666666985	0.000000000
0.125000000	0.666666985	0.139621004
0.128546998	0.666814983	0.278802991
0.375483006	0.832998991	0.209308997
0.375000000	0.833333015	0.069811001
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0.625000000	0.666666985	0.139621004
0.622340977	0.667443991	0.275754005
0.876465023	0.834037006	0.209166005
0.875000000	0.833333015	0.069811001
0.868291020	0.837530971	0.353404999

HCO<sub>2</sub>\*

9.1000003815	0.000000000	0.000000000
0.000000000	9.6520099640	0.000000000
0.000000000	0.000000000	23.0433406830

B	P	O	H	C
36	36	2	1	1

Direct

0.000000000	0.000000000	0.103908002
0.002911000	0.999984980	0.244086996
0.977809012	0.999952018	0.366158009
0.250000000	0.166666999	0.034097001
0.257802010	0.168772995	0.315512002
0.250000000	0.166666999	0.173718005
0.500000000	0.000000000	0.103908002
0.499738991	0.999975979	0.243121997
0.476161987	0.999962986	0.369917005
0.750000000	0.166666999	0.034097001
0.747561991	0.167945996	0.312220007
0.750000000	0.166666999	0.173718005
0.000000000	0.333332986	0.103908002
0.000272000	0.332161009	0.242925003
0.972096980	0.329504013	0.367163986
0.250000000	0.500000000	0.034097001
0.249870002	0.499956012	0.310824007
0.250000000	0.500000000	0.173718005
0.500000000	0.333332986	0.103908002
0.498555005	0.333155006	0.242261007
0.506618023	0.345281988	0.382578999
0.750000000	0.500000000	0.034097001
0.744394004	0.499967009	0.307655007
0.750000000	0.500000000	0.173718005
0.000000000	0.666666985	0.103908002
0.000281000	0.667792976	0.242926002
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0.257795990	0.831166983	0.315506011

0.250000000	0.833333015	0.173718005
0.500000000	0.666666985	0.103908002
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0.750000000	0.833333015	0.034097001
0.747555017	0.831977010	0.312218010
0.750000000	0.833333015	0.173718005
0.125000000	0.000000000	0.034097001
0.125000000	0.000000000	0.173718005
0.137187004	0.999975026	0.314276010
0.375957996	0.166894004	0.243315995
0.375000000	0.166666999	0.103908002
0.381787986	0.170999005	0.388853997
0.625000000	0.000000000	0.034097001
0.625000000	0.000000000	0.173718005
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0.125000000	0.333332986	0.173718005
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0.375000000	0.500000000	0.103908002
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0.625000000	0.333332986	0.173718005
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0.875000000	0.500000000	0.103908002

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0.125000000	0.666666985	0.173718005
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0.375000000	0.833333015	0.103908002
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0.625000000	0.666666985	0.173718005
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0.613045990	0.375559986	0.429778993
0.737318993	0.499981999	0.479932010
0.683802009	0.499947011	0.437287003

H<sub>2</sub>CO<sub>2</sub>\*

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	P	H	O	C
36	36	2	2	1

Direct

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0.250000000	0.166666999	0.173718005



0.500000000	0.000000000	0.103908002
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0.750000000	0.166666999	0.173718005
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0.250000000	0.500000000	0.173718005
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0.750000000	0.500000000	0.173718005
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0.250000000	0.833333015	0.173718005
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0.750000000	0.833333015	0.173718005

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0.125000000	0.000000000	0.173718005
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0.375000000	0.166666999	0.103908002
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0.625000000	0.000000000	0.173718005
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0.875000000	0.166666999	0.103908002
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0.125000000	0.333332986	0.173718005
0.133064002	0.331306010	0.311129987
0.378419012	0.499983013	0.240648001
0.375000000	0.500000000	0.103908002
0.373459011	0.499974012	0.373221010
0.625000000	0.333332986	0.034097001
0.625000000	0.333332986	0.173718005
0.622367978	0.334109008	0.312610000
0.874498010	0.499983013	0.243411005
0.875000000	0.500000000	0.103908002
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0.125000000	0.666666985	0.034097001
0.125000000	0.666666985	0.173718005
0.133064002	0.668623984	0.311116993
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0.375000000	0.833333015	0.103908002
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0.625000000	0.666666985	0.034097001
0.625000000	0.666666985	0.173718005
0.622344017	0.665834010	0.312628001
0.874832988	0.833169997	0.243286997
0.875000000	0.833333015	0.103908002
0.873718023	0.833213985	0.385208994
0.457464010	0.499817014	0.482264996
0.653165996	0.499945015	0.500737011
0.592366993	0.626330972	0.434424013
0.592489004	0.373582989	0.434386998
0.572359979	0.499927014	0.465480000

H<sub>2</sub>CO<sub>2</sub>H\*

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	P	H	O	C
36	36	3	2	1

Direct

0.000000000	0.000000000	0.103908002
0.000379000	0.999656975	0.243456006
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0.250000000	0.166666999	0.034097001
0.254860997	0.167046994	0.313057989
0.250000000	0.166666999	0.173718005
0.500000000	0.000000000	0.103908002
0.500989020	0.000109000	0.242942005
0.472620994	0.996608019	0.369215995
0.750000000	0.166666999	0.034097001
0.746569991	0.167680994	0.313380003
0.750000000	0.166666999	0.173718005

0.000000000	0.333332986	0.103908002
0.998431027	0.332001001	0.242516994
0.976688981	0.332614005	0.366257995
0.250000000	0.500000000	0.034097001
0.248399004	0.499686986	0.308191001
0.250000000	0.500000000	0.173718005
0.500000000	0.333332986	0.103908002
0.500694990	0.333182991	0.243261993
0.491894007	0.339242011	0.384180993
0.750000000	0.500000000	0.034097001
0.747030973	0.499462008	0.311630011
0.750000000	0.500000000	0.173718005
0.000000000	0.666666985	0.103908002
0.998772025	0.667554021	0.242400005
0.980732977	0.669852018	0.364253998
0.250000000	0.833333015	0.034097001
0.257705003	0.833016992	0.313569009
0.250000000	0.833333015	0.173718005
0.500000000	0.666666985	0.103908002
0.500382006	0.666510999	0.242973998
0.494875997	0.656005979	0.381312013
0.750000000	0.833333015	0.034097001
0.747708023	0.831573009	0.312601000
0.750000000	0.833333015	0.173718005
0.125000000	0.000000000	0.034097001
0.125000000	0.000000000	0.173718005
0.134262994	0.999602973	0.312575012
0.377402008	0.166637003	0.242835000
0.375000000	0.166666999	0.103908002
0.371306986	0.164671004	0.386972994

0.625000000	0.000000000	0.034097001
0.625000000	0.000000000	0.173718005
0.627799988	0.999202013	0.313416988
0.874457002	0.166227996	0.243371993
0.875000000	0.166666999	0.103908002
0.872348011	0.166985005	0.386487991
0.125000000	0.333332986	0.034097001
0.125000000	0.333332986	0.173718005
0.130135998	0.332289010	0.311008990
0.377824008	0.499662995	0.241171002
0.375000000	0.500000000	0.103908002
0.361764014	0.498908997	0.377097011
0.625000000	0.333332986	0.034097001
0.625000000	0.333332986	0.173718005
0.622151017	0.333700001	0.313311011
0.875621974	0.499478012	0.242750004
0.875000000	0.500000000	0.103908002
0.878099024	0.503865004	0.383534998
0.125000000	0.666666985	0.034097001
0.125000000	0.666666985	0.173718005
0.133637995	0.668704987	0.310077995
0.377961010	0.833651006	0.242872000
0.375000000	0.833333015	0.103908002
0.373474985	0.828687012	0.389261007
0.625000000	0.666666985	0.034097001
0.625000000	0.666666985	0.173718005
0.623780012	0.665174007	0.312476009
0.875084996	0.833328009	0.243018001
0.875000000	0.833333015	0.103908002
0.874557972	0.833500981	0.385412991

0.446725011	0.494839013	0.483029008
0.640963018	0.482344002	0.504576981
0.700727999	0.599740982	0.424102008
0.593474984	0.616187990	0.436084002
0.583369017	0.363801003	0.436087012
0.561272025	0.479157001	0.468934000

H<sub>2</sub>CO\*+H<sub>2</sub>O\*

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	P	H	O	C
36	36	4	2	1

Direct

0.000000000	0.000000000	0.103909999
0.999390006	0.000330000	0.242689997
0.975070000	0.998820007	0.366549999
0.250000000	0.166669995	0.034100000
0.253060013	0.166590005	0.312909991
0.250000000	0.166669995	0.173720002
0.500000000	0.000000000	0.103909999
0.499480009	0.000080000	0.242689997
0.470539987	0.002540000	0.367659986
0.750000000	0.166669995	0.034100000
0.747569978	0.168290004	0.311140001
0.750000000	0.166669995	0.173720002
0.000000000	0.333330005	0.103909999
0.999750018	0.333469987	0.242709994
0.976220012	0.332850009	0.365889996
0.250000000	0.500000000	0.034100000
0.253639996	0.499480009	0.312750012

0.250000000	0.500000000	0.173720002
0.500000000	0.333330005	0.103909999
0.499460012	0.333440006	0.242359996
0.496800005	0.334789991	0.379550010
0.750000000	0.500000000	0.034100000
0.747300029	0.500140011	0.310920000
0.750000000	0.500000000	0.173720002
0.000000000	0.666670024	0.103909999
0.999670029	0.666790009	0.242819995
0.975269973	0.667919993	0.366759986
0.250000000	0.833329976	0.034100000
0.250090003	0.833519995	0.312189996
0.250000000	0.833329976	0.173720002
0.500000000	0.666670024	0.103909999
0.500479996	0.666880012	0.243300006
0.494269997	0.668370008	0.380169988
0.750000000	0.833329976	0.034100000
0.748319983	0.833079994	0.312319994
0.750000000	0.833329976	0.173720002
0.125000000	0.000000000	0.034100000
0.125000000	0.000000000	0.173720002
0.129930004	0.000780000	0.311919987
0.376379997	0.166730002	0.242829993
0.375000000	0.166669995	0.103909999
0.368420005	0.168789998	0.387809992
0.625000000	0.000000000	0.034100000
0.625000000	0.000000000	0.173720002
0.627370000	0.000510000	0.312869996
0.875940025	0.166899994	0.242699996
0.875000000	0.166669995	0.103909999

0.871309996	0.166800007	0.385619998
0.125000000	0.333330005	0.034100000
0.125000000	0.333330005	0.173720002
0.131640002	0.333160013	0.311800003
0.376650006	0.500220001	0.242670000
0.375000000	0.500000000	0.103909999
0.368189991	0.499949992	0.385080010
0.625000000	0.333330005	0.034100000
0.625000000	0.333330005	0.173720002
0.623420000	0.334149987	0.311080009
0.876139998	0.500310004	0.242719993
0.875000000	0.500000000	0.103909999
0.872150004	0.499170005	0.385049999
0.125000000	0.666670024	0.034100000
0.125000000	0.666670024	0.173720002
0.130510002	0.665719986	0.312139988
0.376230001	0.833260000	0.242860004
0.375000000	0.833329976	0.103909999
0.365700006	0.835590005	0.385470003
0.625000000	0.666670024	0.034100000
0.625000000	0.666670024	0.173720002
0.624949992	0.667119980	0.312949985
0.875760019	0.833509982	0.243139997
0.875000000	0.833329976	0.103909999
0.870639980	0.833599985	0.387050003
0.585250020	0.663200021	0.523949981
0.396800011	0.676639974	0.486420006
0.675320029	0.253320009	0.431160003
0.680679977	0.416680008	0.428700000
0.583869994	0.665099978	0.436470002



0.606980026	0.336829990	0.433999985
0.516939998	0.668150008	0.484899998

H<sub>2</sub>CO\*

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	P	H	C	O
36	36	3	1	1

Direct

0.000000000	0.000000000	0.103908002
0.999296010	0.000040000	0.242763996
0.976006985	0.000563000	0.365458995
0.250000000	0.166666999	0.034097001
0.251433998	0.166754007	0.311733007
0.250000000	0.166666999	0.173718005
0.500000000	0.000000000	0.103908002
0.500105023	0.000003000	0.242595002
0.470679998	0.000874000	0.366961002
0.750000000	0.166666999	0.034097001
0.748713017	0.166988000	0.312442988
0.750000000	0.166666999	0.173718005
0.000000000	0.333332986	0.103908002
0.999315977	0.333460003	0.242789000
0.975705981	0.333196014	0.365612000
0.250000000	0.500000000	0.034097001
0.252884001	0.499821991	0.312249005
0.250000000	0.500000000	0.173718005
0.500000000	0.333332986	0.103908002
0.500262022	0.333597988	0.242631003
0.470373988	0.332791001	0.367224008

0.750000000	0.500000000	0.034097001
0.747272015	0.501145005	0.312878013
0.750000000	0.500000000	0.173718005
0.000000000	0.666666985	0.103908002
0.999679983	0.666760981	0.243009001
0.975522995	0.667086005	0.365958989
0.250000000	0.833333015	0.034097001
0.252557009	0.833347023	0.311987013
0.250000000	0.833333015	0.173718005
0.500000000	0.666666985	0.103908002
0.500407994	0.666767001	0.243107006
0.503337979	0.662856996	0.384182006
0.750000000	0.833333015	0.034097001
0.747278988	0.832477987	0.312887996
0.750000000	0.833333015	0.173718005
0.125000000	0.000000000	0.034097001
0.125000000	0.000000000	0.173718005
0.131049007	0.000099000	0.311473012
0.377005011	0.166859999	0.242574006
0.375000000	0.166666999	0.103908002
0.366216004	0.166798994	0.387571990
0.625000000	0.000000000	0.034097001
0.625000000	0.000000000	0.173718005
0.627678990	0.000290000	0.312525004
0.875539005	0.166768998	0.242937997
0.875000000	0.166666999	0.103908002
0.871909976	0.166795999	0.386016995
0.125000000	0.333332986	0.034097001
0.125000000	0.333332986	0.173718005
0.130795002	0.333750010	0.311536014

0.376913011	0.500199974	0.242594004
0.375000000	0.500000000	0.103908002
0.367022008	0.498136014	0.385910004
0.625000000	0.333332986	0.034097001
0.625000000	0.333332986	0.173718005
0.627376020	0.333626986	0.312768996
0.875099003	0.500478983	0.243168995
0.875000000	0.500000000	0.103908002
0.872206986	0.499978989	0.385376990
0.125000000	0.666666985	0.034097001
0.125000000	0.666666985	0.173718005
0.131550997	0.666486979	0.312090993
0.377048999	0.833308995	0.242420003
0.375000000	0.833333015	0.103908002
0.370389014	0.834040999	0.384216011
0.625000000	0.666666985	0.034097001
0.625000000	0.666666985	0.173718005
0.622618973	0.667183995	0.312505007
0.875124991	0.833185017	0.243193999
0.875000000	0.833333015	0.103908002
0.872659028	0.834267020	0.385506004
0.464482009	0.728794992	0.498968005
0.646986008	0.673330009	0.518339992
0.510474026	0.548089027	0.497263998
0.553057015	0.653581023	0.489596993
0.602519989	0.669102013	0.431391001

H<sub>2</sub>COH\*

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	P	H	C	O
36	36	4	1	1

Direct

0.000000000	0.000000000	0.103908002
0.999656975	0.999390006	0.242805004
0.975881994	0.001496000	0.366191000
0.250000000	0.166666999	0.034097001
0.249215007	0.167086005	0.311966985
0.250000000	0.166666999	0.173718005
0.500000000	0.000000000	0.103908002
0.499848992	0.000007000	0.242831007
0.472000003	0.997183025	0.367437989
0.750000000	0.166666999	0.034097001
0.749166012	0.166118994	0.312417001
0.750000000	0.166666999	0.173718005
0.000000000	0.333332986	0.103908002
0.998808026	0.332789987	0.242446005
0.973532021	0.332630992	0.367096007
0.250000000	0.500000000	0.034097001
0.250032991	0.499246001	0.311688989
0.250000000	0.500000000	0.173718005
0.500000000	0.333332986	0.103908002
0.499624997	0.333245009	0.242625996
0.470299006	0.330969989	0.366573989
0.750000000	0.500000000	0.034097001
0.748243988	0.500680029	0.311022013
0.750000000	0.500000000	0.173718005
0.000000000	0.666666985	0.103908002
0.999665976	0.666756988	0.242642000
0.976270974	0.669511974	0.365999013

0.250000000	0.833333015	0.034097001
0.253244013	0.833124995	0.313093007
0.250000000	0.833333015	0.173718005
0.500000000	0.666666985	0.103908002
0.499920994	0.666481018	0.242888004
0.495613009	0.661485016	0.379691005
0.750000000	0.833333015	0.034097001
0.748371005	0.831672013	0.312265009
0.750000000	0.833333015	0.173718005
0.125000000	0.000000000	0.034097001
0.125000000	0.000000000	0.173718005
0.130787000	0.999530017	0.312013000
0.376112998	0.166806996	0.242865995
0.375000000	0.166666999	0.103908002
0.367361009	0.164370000	0.386970013
0.625000000	0.000000000	0.034097001
0.625000000	0.000000000	0.173718005
0.628131986	0.998991013	0.312914997
0.875633001	0.166044995	0.243009999
0.875000000	0.166666999	0.103908002
0.869889021	0.166562006	0.387479991
0.125000000	0.333332986	0.034097001
0.125000000	0.333332986	0.173718005
0.127664000	0.333813012	0.311782986
0.376190007	0.499924004	0.242633000
0.375000000	0.500000000	0.103908002
0.364740014	0.496612996	0.385078996
0.625000000	0.333332986	0.034097001
0.625000000	0.333332986	0.173718005
0.628076017	0.332699001	0.312684000

0.876164973	0.499805987	0.242580995
0.875000000	0.500000000	0.103908002
0.871721983	0.502601981	0.385342985
0.125000000	0.666666985	0.034097001
0.125000000	0.666666985	0.173718005
0.131160006	0.667020977	0.311800003
0.376560986	0.833185017	0.242946997
0.375000000	0.833333015	0.103908002
0.370072007	0.830555975	0.387459010
0.625000000	0.666666985	0.034097001
0.625000000	0.666666985	0.173718005
0.624019027	0.666046977	0.312128007
0.875606000	0.832949996	0.243031994
0.875000000	0.833333015	0.103908002
0.872433007	0.835125029	0.386377990
0.499828011	0.527336001	0.496805996
0.455745995	0.709212005	0.498071015
0.634516001	0.651871026	0.522625983
0.689647019	0.587419987	0.426351994
0.543604016	0.632822990	0.492489994
0.601840019	0.653289974	0.433937013

\*OH

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	P	H	O
36	36	1	1

Direct

0.000000000	0.000000000	0.103908002
0.999440014	0.999704003	0.242921993

0.975840986	0.000467000	0.365696996
0.250000000	0.166666999	0.034097001
0.250676990	0.167076007	0.311863989
0.250000000	0.166666999	0.173718005
0.500000000	0.000000000	0.103908002
0.500093997	0.999966025	0.242771000
0.470901012	0.001416000	0.367579997
0.750000000	0.166666999	0.034097001
0.749198973	0.166374996	0.312492996
0.750000000	0.166666999	0.173718005
0.000000000	0.333332986	0.103908002
0.999162018	0.333492994	0.242800996
0.974961996	0.332973003	0.366129011
0.250000000	0.500000000	0.034097001
0.252651989	0.500029981	0.311944991
0.250000000	0.500000000	0.173718005
0.500000000	0.333332986	0.103908002
0.500037014	0.333272994	0.242578000
0.471248001	0.331773996	0.366845012
0.750000000	0.500000000	0.034097001
0.746707976	0.501389027	0.312386990
0.750000000	0.500000000	0.173718005
0.000000000	0.666666985	0.103908002
0.999650002	0.666764021	0.243042007
0.975574970	0.667141020	0.366007000
0.250000000	0.833333015	0.034097001
0.253208011	0.833589017	0.312519014
0.250000000	0.833333015	0.173718005
0.500000000	0.666666985	0.103908002
0.499902010	0.666615009	0.243064001

0.502300978	0.670823991	0.386141002
0.750000000	0.833333015	0.034097001
0.746501029	0.832117021	0.313080996
0.750000000	0.833333015	0.173718005
0.125000000	0.000000000	0.034097001
0.125000000	0.000000000	0.173718005
0.131178007	0.999733984	0.311760992
0.376637995	0.166648000	0.242690995
0.375000000	0.166666999	0.103908002
0.366420001	0.166996002	0.387445003
0.625000000	0.000000000	0.034097001
0.625000000	0.000000000	0.173718005
0.627505004	0.999954998	0.312900990
0.875824988	0.166452006	0.242951006
0.875000000	0.166666999	0.103908002
0.871432006	0.166466996	0.386440992
0.125000000	0.333332986	0.034097001
0.125000000	0.333332986	0.173718005
0.130210996	0.333763003	0.311812997
0.377005011	0.499902010	0.242329001
0.375000000	0.500000000	0.103908002
0.373263001	0.499529004	0.383648008
0.625000000	0.333332986	0.034097001
0.625000000	0.333332986	0.173718005
0.628247976	0.332942992	0.312361985
0.875213027	0.500386000	0.243040994
0.875000000	0.500000000	0.103908002
0.871644020	0.500226021	0.385711998
0.125000000	0.666666985	0.034097001
0.125000000	0.666666985	0.173718005



0.131692007	0.666921020	0.312211990
0.376783997	0.833271980	0.242649004
0.375000000	0.833333015	0.103908002
0.369915009	0.835011005	0.385688990
0.625000000	0.666666985	0.034097001
0.625000000	0.666666985	0.173718005
0.621814013	0.666347027	0.312373996
0.874868989	0.832835019	0.243248001
0.875000000	0.833333015	0.103908002
0.872426987	0.833886981	0.385416001
0.659726977	0.597092986	0.439686000
0.592889011	0.676488996	0.435988009

H<sub>2</sub>O\*

9.1000003815	0.0000000000	0.0000000000
0.0000000000	9.6520099640	0.0000000000
0.0000000000	0.0000000000	23.0433406830

B	P	H	O
36	36	2	1

Direct

0.000000000	0.000000000	0.103908002
0.999737024	0.999840975	0.242737994
0.974029005	0.001520000	0.367036998
0.250000000	0.166666999	0.034097001
0.249005005	0.166624993	0.312328994
0.250000000	0.166666999	0.173718005
0.500000000	0.000000000	0.103908002
0.499383003	0.000021000	0.242705002
0.471868008	0.999216020	0.367074013
0.750000000	0.166666999	0.034097001
0.749351978	0.166562006	0.312299013

0.750000000	0.166666999	0.173718005
0.000000000	0.333332986	0.103908002
0.999747992	0.333409995	0.242712006
0.974002004	0.331761003	0.366979986
0.250000000	0.500000000	0.034097001
0.252393991	0.499819994	0.313059002
0.250000000	0.500000000	0.173718005
0.500000000	0.333332986	0.103908002
0.499343991	0.333260000	0.242704004
0.471830010	0.333606988	0.366991013
0.750000000	0.500000000	0.034097001
0.748362005	0.501091003	0.310880989
0.750000000	0.500000000	0.173718005
0.000000000	0.666666985	0.103908002
0.000223000	0.666616023	0.242750004
0.975093007	0.666751981	0.366465002
0.250000000	0.833333015	0.034097001
0.252402991	0.833425999	0.313115001
0.250000000	0.833333015	0.173718005
0.500000000	0.666666985	0.103908002
0.499410987	0.666655004	0.242393002
0.498376995	0.666233003	0.379141986
0.750000000	0.833333015	0.034097001
0.748250008	0.832038999	0.310867995
0.750000000	0.833333015	0.173718005
0.125000000	0.000000000	0.034097001
0.125000000	0.000000000	0.173718005
0.129175007	0.999228001	0.312366992
0.375631005	0.166612998	0.242963001
0.375000000	0.166666999	0.103908002

0.368124992	0.166449994	0.386911988
0.625000000	0.000000000	0.034097001
0.625000000	0.000000000	0.173718005
0.628162980	0.999747992	0.312548995
0.876091003	0.166620001	0.243033007
0.875000000	0.166666999	0.103908002
0.868902981	0.166640997	0.387831986
0.125000000	0.333332986	0.034097001
0.125000000	0.333332986	0.173718005
0.129163995	0.334021986	0.312348008
0.375995994	0.500042975	0.242916003
0.375000000	0.500000000	0.103908002
0.369810998	0.500150025	0.387053996
0.625000000	0.333332986	0.034097001
0.625000000	0.333332986	0.173718005
0.628257990	0.333359003	0.312534004
0.876540005	0.499967009	0.242588997
0.875000000	0.500000000	0.103908002
0.870600998	0.500096023	0.385668993
0.125000000	0.666666985	0.034097001
0.125000000	0.666666985	0.173718005
0.130925000	0.666646004	0.312370002
0.375912994	0.833275020	0.242924005
0.375000000	0.833333015	0.103908002
0.370005012	0.832583010	0.387124002
0.625000000	0.666666985	0.034097001
0.625000000	0.666666985	0.173718005
0.624059975	0.666525006	0.310921997
0.876477003	0.833229005	0.242609993
0.875000000	0.833333015	0.103908002

0.870366991	0.833232999	0.385704011
0.676685989	0.583777010	0.430496991
0.676243007	0.747682989	0.430929005
0.605876029	0.665601015	0.433955014

**The coordinates files of CH<sub>4</sub> formation on BAs (110)**

CO<sub>2</sub>\*

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	H	O
36	36	2	1

Direct

0.000000000	0.000000000	0.099382997
0.970685005	0.998594999	0.378526986
0.250000000	0.166669995	0.025953000
0.253459990	0.166427001	0.321985990
0.250000000	0.166669995	0.172812998
0.000510000	0.000178000	0.246441007
0.500000000	0.000000000	0.099382997
0.469040990	0.000694000	0.378592998
0.750000000	0.166669995	0.025953000
0.749031007	0.168119997	0.319501013
0.750000000	0.166669995	0.172812998
0.500212014	0.000049000	0.246400997
0.000000000	0.333330005	0.099382997
0.972348988	0.333723992	0.377804011
0.250000000	0.500000000	0.025953000
0.253291011	0.500602007	0.321891993
0.250000000	0.500000000	0.172812998

0.001014000	0.333415985	0.246489003
0.500000000	0.333330005	0.099382997
0.496769011	0.333537012	0.391719013
0.750000000	0.500000000	0.025953000
0.748969018	0.498843998	0.319453001
0.750000000	0.500000000	0.172812998
0.500015020	0.333460003	0.246197000
0.000000000	0.666670024	0.099382997
0.970808029	0.668706000	0.378515005
0.250000000	0.833329976	0.025953000
0.249556005	0.833519995	0.321006000
0.250000000	0.833329976	0.172812998
0.000480000	0.666697979	0.246414006
0.500000000	0.666670024	0.099382997
0.468901008	0.666336000	0.378564000
0.750000000	0.833329976	0.025953000
0.750047982	0.833459020	0.320787996
0.750000000	0.833329976	0.172812998
0.500065982	0.666844010	0.246391997
0.125000000	0.000000000	0.172812998
0.127734005	0.000964000	0.320739001
0.125000000	0.000000000	0.025953000
0.375562996	0.166693002	0.246949002
0.375000000	0.166669995	0.099382997
0.365758985	0.167355999	0.402485013
0.625000000	0.000000000	0.172812998
0.626960993	0.000329000	0.320865005
0.625000000	0.000000000	0.025953000
0.876188993	0.166795000	0.246603996
0.875000000	0.166669995	0.099382997

0.866671979	0.167297006	0.400595009
0.125000000	0.333330005	0.172812998
0.130128995	0.333516002	0.320656002
0.125000000	0.333330005	0.025953000
0.375528008	0.500205994	0.246913001
0.375000000	0.500000000	0.099382997
0.365671009	0.499605000	0.402379006
0.625000000	0.333330005	0.172812998
0.623097003	0.333438993	0.319348991
0.625000000	0.333330005	0.025953000
0.876222014	0.500055015	0.246601999
0.875000000	0.500000000	0.099382997
0.866685987	0.500153005	0.400566995
0.125000000	0.666670024	0.172812998
0.127712995	0.666119993	0.320686996
0.125000000	0.666670024	0.025953000
0.375220001	0.833467007	0.247001007
0.375000000	0.833329976	0.099382997
0.363656998	0.833545029	0.402213991
0.625000000	0.666670024	0.172812998
0.626811981	0.666656017	0.320809007
0.625000000	0.666670024	0.025953000
0.875787973	0.833432019	0.246996999
0.875000000	0.833329976	0.099382997
0.863937020	0.833563030	0.403061986
0.665925980	0.412169009	0.444521010
0.666779995	0.255856991	0.444317013
0.600233018	0.333683014	0.446455002

HCO<sub>2</sub>\*

9.5539999008

0.0000000000

0.0000000000

0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	O	H	C
36	36	2	1	1

Direct

0.0000000000	0.0000000000	0.099380001
0.972389996	0.999989986	0.377260000
0.250000000	0.166669995	0.025950000
0.256650001	0.167229995	0.322479993
0.250000000	0.166669995	0.172810003
0.001030000	0.999989986	0.247199997
0.500000000	0.000000000	0.099380001
0.469249994	0.999989986	0.380329996
0.750000000	0.166669995	0.025950000
0.747759998	0.168750003	0.321689993
0.750000000	0.166669995	0.172810003
0.501770020	0.000000000	0.246739998
0.000000000	0.333330005	0.099380001
0.974380016	0.330900013	0.376300007
0.250000000	0.500000000	0.025950000
0.246470004	0.500000000	0.316579998
0.250000000	0.500000000	0.172810003
0.998629987	0.331750005	0.245619997
0.500000000	0.333330005	0.099380001
0.488730013	0.349959999	0.393599987
0.750000000	0.500000000	0.025950000
0.749109983	0.499989986	0.320259988
0.750000000	0.500000000	0.172810003
0.501169980	0.333600014	0.246959999
0.000000000	0.666670024	0.099380001

0.974380016	0.669070005	0.376300007
0.250000000	0.833329976	0.025950000
0.256650001	0.832759976	0.322479993
0.250000000	0.833329976	0.172810003
0.998629987	0.668240011	0.245619997
0.500000000	0.666670024	0.099380001
0.488730013	0.650020003	0.393599987
0.750000000	0.833329976	0.025950000
0.747759998	0.831239998	0.321689993
0.750000000	0.833329976	0.172810003
0.501169980	0.666390002	0.246959999
0.125000000	0.000000000	0.172810003
0.132269993	0.999989986	0.321049988
0.125000000	0.000000000	0.025950000
0.377000004	0.166590005	0.246979997
0.375000000	0.166669995	0.099380001
0.368470013	0.170369998	0.403360009
0.625000000	0.000000000	0.172810003
0.626540005	0.999989986	0.321649998
0.625000000	0.000000000	0.025950000
0.873769999	0.166290000	0.247209996
0.875000000	0.166669995	0.099380001
0.867330015	0.166710004	0.401639998
0.125000000	0.333330005	0.172810003
0.128859997	0.331559986	0.318010002
0.125000000	0.333330005	0.025950000
0.376340002	0.500000000	0.245580003
0.375000000	0.500000000	0.099380001
0.339670002	0.499989986	0.395460010
0.625000000	0.333330005	0.172810003



0.621290028	0.335399985	0.321759999
0.625000000	0.333330005	0.025950000
0.875240028	0.500000000	0.246590003
0.875000000	0.500000000	0.099380001
0.874480009	0.499989986	0.398620009
0.125000000	0.666670024	0.172810003
0.128849998	0.668429971	0.318010002
0.125000000	0.666670024	0.025950000
0.377000004	0.833400011	0.246979997
0.375000000	0.833329976	0.099380001
0.368470013	0.829620004	0.403360009
0.625000000	0.666670024	0.172810003
0.621290028	0.664590001	0.321759999
0.625000000	0.666670024	0.025950000
0.873769999	0.833700001	0.247209996
0.875000000	0.833329976	0.099380001
0.867330015	0.833260000	0.401639998
0.579020023	0.616060019	0.445809990
0.579020023	0.383920014	0.445809990
0.677690029	0.499989986	0.503849983
0.616550028	0.499989986	0.463739991

H<sub>2</sub>CO<sub>2</sub>\*

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	H	O	C
36	36	2	2	1

Direct

0.000000000	0.000000000	0.099380001
0.972249985	0.000130000	0.376839995

0.250000000	0.166669995	0.025950000
0.257569999	0.166989997	0.322310001
0.250000000	0.166669995	0.172810003
0.000920000	0.000100000	0.247140005
0.500000000	0.000000000	0.099380001
0.471700013	0.000220000	0.378879994
0.750000000	0.166669995	0.025950000
0.747929990	0.168950006	0.321530014
0.750000000	0.166669995	0.172810003
0.501670003	0.000080000	0.246309996
0.000000000	0.333330005	0.099380001
0.973749995	0.331930012	0.376219988
0.250000000	0.500000000	0.025950000
0.248930007	0.500150025	0.317189991
0.250000000	0.500000000	0.172810003
0.999119997	0.332280010	0.246169999
0.500000000	0.333330005	0.099380001
0.497350007	0.354039997	0.398499995
0.750000000	0.500000000	0.025950000
0.747449994	0.500129998	0.321740001
0.750000000	0.500000000	0.172810003
0.501060009	0.333510011	0.247020006
0.000000000	0.666670024	0.099380001
0.973789990	0.668330014	0.376199991
0.250000000	0.833329976	0.025950000
0.257580012	0.833329976	0.322320014
0.250000000	0.833329976	0.172810003
0.999090016	0.667869985	0.246179998
0.500000000	0.666670024	0.099380001
0.497370005	0.646679997	0.398460001

0.750000000	0.833329976	0.025950000
0.747959971	0.831309974	0.321500003
0.750000000	0.833329976	0.172810003
0.501070023	0.666649997	0.246969998
0.125000000	0.000000000	0.172810003
0.132149994	0.000150000	0.320879996
0.125000000	0.000000000	0.025950000
0.377130002	0.166529998	0.246739998
0.375000000	0.166669995	0.099380001
0.368959993	0.167089999	0.402810007
0.625000000	0.000000000	0.172810003
0.628000021	0.000130000	0.320520014
0.625000000	0.000000000	0.025950000
0.874379992	0.166740000	0.247060001
0.875000000	0.166669995	0.099380001
0.867399991	0.166920006	0.401179999
0.125000000	0.333330005	0.172810003
0.129779994	0.331790000	0.318740010
0.125000000	0.333330005	0.025950000
0.376949996	0.500090003	0.245509997
0.375000000	0.500000000	0.099380001
0.344810009	0.500280023	0.395429999
0.625000000	0.333330005	0.172810003
0.620599985	0.334360003	0.321590006
0.625000000	0.333330005	0.025950000
0.874419987	0.500069976	0.247040004
0.875000000	0.500000000	0.099380001
0.871919990	0.500140011	0.398950011
0.125000000	0.666670024	0.172810003
0.129779994	0.668510020	0.318720013

0.125000000	0.666670024	0.025950000
0.377119988	0.833630025	0.246739998
0.375000000	0.833329976	0.099380001
0.368869990	0.833360016	0.402810007
0.625000000	0.666670024	0.172810003
0.620589972	0.665880024	0.321559995
0.625000000	0.666670024	0.025950000
0.874430001	0.833440006	0.247040004
0.875000000	0.833329976	0.099380001
0.867389977	0.833310008	0.401149988
0.473529994	0.500490010	0.500530005
0.663460016	0.500450015	0.509199977
0.588779986	0.619369984	0.445190012
0.588670015	0.381410003	0.445279986
0.576210022	0.500440001	0.478289992

H<sub>2</sub>CO<sub>2</sub>H\*

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	H	O	C
36	36	3	2	1

Direct

0.000000000	0.000000000	0.099382997
0.971643984	0.001192000	0.377398998
0.250000000	0.166669995	0.025953000
0.255219996	0.167515993	0.322378993
0.250000000	0.166669995	0.172812998
0.000825000	0.999930978	0.247075006
0.500000000	0.000000000	0.099382997
0.468562007	0.999131024	0.380190998

0.750000000	0.166669995	0.025953000
0.747192025	0.168623000	0.321639001
0.750000000	0.166669995	0.172812998
0.501479983	0.000222000	0.246657997
0.000000000	0.333330005	0.099382997
0.972972989	0.332208008	0.377319992
0.250000000	0.500000000	0.025953000
0.247908995	0.499972999	0.316965997
0.250000000	0.500000000	0.172812998
0.998932004	0.331995994	0.245807007
0.500000000	0.333330005	0.099382997
0.490552008	0.347422987	0.396046996
0.750000000	0.500000000	0.025953000
0.748889983	0.499624997	0.320405006
0.750000000	0.500000000	0.172812998
0.501496971	0.333364010	0.247064993
0.000000000	0.666670024	0.099382997
0.977087975	0.668896973	0.375533998
0.250000000	0.833329976	0.025953000
0.256859988	0.833459973	0.322243989
0.250000000	0.833329976	0.172812998
0.998924971	0.667864025	0.245607004
0.500000000	0.666670024	0.099382997
0.489611000	0.653985023	0.393839985
0.750000000	0.833329976	0.025953000
0.747524023	0.830949008	0.321042001
0.750000000	0.833329976	0.172812998
0.500829995	0.666350007	0.246891007
0.125000000	0.000000000	0.172812998
0.131415993	0.999970973	0.321006000

0.125000000	0.000000000	0.025953000
0.376625001	0.166761994	0.246997997
0.375000000	0.166669995	0.099382997
0.368097991	0.168452993	0.402404010
0.625000000	0.000000000	0.172812998
0.626336992	0.999598980	0.321516991
0.625000000	0.000000000	0.025953000
0.873906016	0.166299000	0.247236997
0.875000000	0.166669995	0.099382997
0.865903974	0.167163000	0.402083993
0.125000000	0.333330005	0.172812998
0.127866000	0.332379997	0.318726987
0.125000000	0.333330005	0.025953000
0.376765013	0.499545991	0.245480001
0.375000000	0.500000000	0.099382997
0.344808012	0.500464976	0.395112991
0.625000000	0.333330005	0.172812998
0.620738983	0.334715992	0.321909010
0.625000000	0.333330005	0.025953000
0.875195026	0.499691010	0.246719003
0.875000000	0.500000000	0.099382997
0.874041975	0.502942026	0.399347991
0.125000000	0.666670024	0.172812998
0.130775005	0.668582976	0.317624986
0.125000000	0.666670024	0.025953000
0.377085000	0.833676994	0.246912003
0.375000000	0.833329976	0.099382997
0.367733985	0.829901993	0.403652996
0.625000000	0.666670024	0.172812998
0.621438980	0.664133012	0.321453005

0.625000000	0.666670024	0.025953000
0.874194026	0.833462000	0.246959999
0.875000000	0.833329976	0.099382997
0.868725002	0.832176983	0.400673002
0.462691009	0.490363985	0.499262989
0.653090000	0.486214995	0.512044013
0.684255004	0.628802001	0.441468000
0.581746995	0.619000971	0.448765010
0.585489988	0.374648988	0.445109010
0.567686975	0.480199993	0.480286986

H<sub>2</sub>CO+H<sub>2</sub>O

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	H	O	C
36	36	4	2	1

Direct

0.000000000	0.000000000	0.099382997
0.971269011	0.001332000	0.378008008
0.250000000	0.166669995	0.025953000
0.250404000	0.166233003	0.321079999
0.250000000	0.166669995	0.172812998
0.000197000	0.999592006	0.246295005
0.500000000	0.000000000	0.099382997
0.468353003	0.997464001	0.379002005
0.750000000	0.166669995	0.025953000
0.749315977	0.167034999	0.320663005
0.750000000	0.166669995	0.172812998
0.500172019	0.999994993	0.246383995
0.000000000	0.333330005	0.099382997

0.971414983	0.331636995	0.378178000
0.250000000	0.500000000	0.025953000
0.254189014	0.500198007	0.321709007
0.250000000	0.500000000	0.172812998
0.000364000	0.333108991	0.246402994
0.500000000	0.333330005	0.099382997
0.494655013	0.330475986	0.393007010
0.750000000	0.500000000	0.025953000
0.748070002	0.499736995	0.319303989
0.750000000	0.500000000	0.172812998
0.501025021	0.333056003	0.247012004
0.000000000	0.666670024	0.099382997
0.973240972	0.667095006	0.377184004
0.250000000	0.833329976	0.025953000
0.253639996	0.833552003	0.321662009
0.250000000	0.833329976	0.172812998
0.000486000	0.666432977	0.246323004
0.500000000	0.666670024	0.099382997
0.495683014	0.664737999	0.391676009
0.750000000	0.833329976	0.025953000
0.748422980	0.831544995	0.319476008
0.750000000	0.833329976	0.172812998
0.499812990	0.666436017	0.246029004
0.125000000	0.000000000	0.172812998
0.128074005	0.999089003	0.320252001
0.125000000	0.000000000	0.025953000
0.375611991	0.166667998	0.246930003
0.375000000	0.166669995	0.099382997
0.361443013	0.163922995	0.400604993
0.625000000	0.000000000	0.172812998



0.626501977	0.999472976	0.321015000
0.625000000	0.000000000	0.025953000
0.875594020	0.166372001	0.246999994
0.875000000	0.166669995	0.099382997
0.865119994	0.166271999	0.402480990
0.125000000	0.333330005	0.172812998
0.128619000	0.334120005	0.320416987
0.125000000	0.333330005	0.025953000
0.376015007	0.499574989	0.246654004
0.375000000	0.500000000	0.099382997
0.365016997	0.499475002	0.399749994
0.625000000	0.333330005	0.172812998
0.624019980	0.332792014	0.321011990
0.625000000	0.333330005	0.025953000
0.875904977	0.499642015	0.246600002
0.875000000	0.500000000	0.099382997
0.868121028	0.500900984	0.399895996
0.125000000	0.666670024	0.172812998
0.130383000	0.666740000	0.320014000
0.125000000	0.666670024	0.025953000
0.375858992	0.833384991	0.246819004
0.375000000	0.833329976	0.099382997
0.364445001	0.830999017	0.402704000
0.625000000	0.666670024	0.172812998
0.622771025	0.665844977	0.319121987
0.625000000	0.666670024	0.025953000
0.875804007	0.833018005	0.246537998
0.875000000	0.833329976	0.099382997
0.867069006	0.832917988	0.400335997
0.423848987	0.314512014	0.505582988

0.612378001	0.338268012	0.533288002
0.665470004	0.742641985	0.444146007
0.671088994	0.586816013	0.441498995
0.601675987	0.662783027	0.445825994
0.584083021	0.336237997	0.446377009
0.535948992	0.329649001	0.498100996

H<sub>2</sub>CO

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	H	C	O
36	36	2	1	1

Direct

0.000000000	0.000000000	0.099382997
0.971045017	0.999816000	0.377398014
0.250000000	0.166669995	0.025953000
0.251289010	0.166199997	0.320629001
0.250000000	0.166669995	0.172812998
0.999684989	0.999953985	0.246156007
0.500000000	0.000000000	0.099382997
0.468663007	0.999979019	0.378257990
0.750000000	0.166669995	0.025953000
0.749261975	0.167842001	0.320793986
0.750000000	0.166669995	0.172812998
0.500411987	0.000022000	0.246338993
0.000000000	0.333330005	0.099382997
0.971159995	0.333566993	0.377496004
0.250000000	0.500000000	0.025953000
0.251062989	0.500523984	0.320695013
0.250000000	0.500000000	0.172812998

0.000011000	0.333281994	0.246291995
0.500000000	0.333330005	0.099382997
0.495274991	0.334401995	0.392324001
0.750000000	0.500000000	0.025953000
0.749405980	0.499128014	0.320706010
0.750000000	0.500000000	0.172812998
0.501178980	0.333353996	0.246913999
0.000000000	0.666670024	0.099382997
0.971008003	0.667325020	0.377469003
0.250000000	0.833329976	0.025953000
0.250344008	0.833319008	0.320302010
0.250000000	0.833329976	0.172812998
0.999596000	0.666756988	0.246129006
0.500000000	0.666670024	0.099382997
0.468712002	0.667532027	0.378311992
0.750000000	0.833329976	0.025953000
0.749688983	0.833405972	0.320980012
0.750000000	0.833329976	0.172812998
0.500355005	0.666522026	0.246341005
0.125000000	0.000000000	0.172812998
0.127684996	0.999963999	0.319891989
0.125000000	0.000000000	0.025953000
0.376262009	0.166746005	0.246691003
0.375000000	0.166669995	0.099382997
0.362987995	0.166471004	0.400186002
0.625000000	0.000000000	0.172812998
0.626820028	0.000364000	0.320820004
0.625000000	0.000000000	0.025953000
0.875136018	0.166633993	0.246941000
0.875000000	0.166669995	0.099382997

0.866589010	0.166486993	0.401683003
0.125000000	0.333330005	0.172812998
0.128529996	0.333337992	0.320122987
0.125000000	0.333330005	0.025953000
0.376064003	0.499834001	0.246736005
0.375000000	0.500000000	0.099382997
0.362197995	0.501523018	0.400370002
0.625000000	0.333330005	0.172812998
0.624191999	0.333550006	0.320753992
0.625000000	0.333330005	0.025953000
0.875173986	0.500006974	0.246868998
0.875000000	0.500000000	0.099382997
0.866397977	0.500563979	0.401591986
0.125000000	0.666670024	0.172812998
0.127478004	0.666724026	0.319880009
0.125000000	0.666670024	0.025953000
0.376118988	0.833280981	0.246714994
0.375000000	0.833329976	0.099382997
0.362457007	0.833666027	0.402440012
0.625000000	0.666670024	0.172812998
0.626914024	0.666540027	0.320852995
0.625000000	0.666670024	0.025953000
0.875042021	0.833374023	0.246888995
0.875000000	0.833329976	0.099382997
0.865674019	0.833585978	0.402157992
0.425738990	0.342352003	0.505733013
0.616692007	0.332446992	0.532132030
0.538578987	0.335750014	0.497451991
0.584743977	0.332475990	0.445643991

H<sub>3</sub>CO

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	H	C	O
36	36	3	1	1

Direct

0.000000000	0.000000000	0.099382997
0.971354008	0.000171000	0.377018988
0.250000000	0.166669995	0.025953000
0.252124995	0.166736007	0.321052998
0.250000000	0.166669995	0.172812998
0.999619007	0.000220000	0.246194005
0.500000000	0.000000000	0.099382997
0.466174990	0.001874000	0.378179997
0.750000000	0.166669995	0.025953000
0.748678982	0.168524995	0.321328014
0.750000000	0.166669995	0.172812998
0.500621974	0.000363000	0.246379003
0.000000000	0.333330005	0.099382997
0.970467985	0.333523005	0.377490997
0.250000000	0.500000000	0.025953000
0.252662987	0.500607014	0.321209013
0.250000000	0.500000000	0.172812998
0.000195000	0.333555996	0.246448994
0.500000000	0.333330005	0.099382997
0.502982020	0.336908013	0.396636009
0.750000000	0.500000000	0.025953000
0.748319983	0.499008000	0.321132004
0.750000000	0.500000000	0.172812998
0.501042008	0.333463997	0.246900007

0.000000000	0.666670024	0.099382997
0.971172988	0.666891992	0.377061993
0.250000000	0.833329976	0.025953000
0.250871003	0.833625972	0.320423990
0.250000000	0.833329976	0.172812998
0.999656975	0.666853011	0.246259004
0.500000000	0.666670024	0.099382997
0.466338009	0.667011023	0.378358990
0.750000000	0.833329976	0.025953000
0.748973012	0.833612978	0.321114987
0.750000000	0.833329976	0.172812998
0.500459015	0.666700006	0.246369004
0.125000000	0.000000000	0.172812998
0.128092006	0.000351000	0.319660991
0.125000000	0.000000000	0.025953000
0.375995010	0.166989997	0.246632993
0.375000000	0.166669995	0.099382997
0.361360013	0.166771993	0.400694996
0.625000000	0.000000000	0.172812998
0.625980973	0.000792000	0.321029007
0.625000000	0.000000000	0.025953000
0.874688029	0.167037994	0.247104004
0.875000000	0.166669995	0.099382997
0.866208971	0.166242003	0.401674002
0.125000000	0.333330005	0.172812998
0.128702998	0.333754987	0.320293009
0.125000000	0.333330005	0.025953000
0.376017988	0.499920011	0.246714994
0.375000000	0.500000000	0.099382997
0.360637993	0.501851022	0.401414007

0.625000000	0.333330005	0.172812998
0.621563971	0.333411008	0.321063012
0.625000000	0.333330005	0.025953000
0.874656975	0.499926001	0.247048005
0.875000000	0.500000000	0.099382997
0.865664005	0.500688016	0.401394993
0.125000000	0.666670024	0.172812998
0.128188998	0.666517019	0.319739997
0.125000000	0.666670024	0.025953000
0.376129001	0.833482027	0.246648997
0.375000000	0.833329976	0.099382997
0.361221999	0.834114015	0.402366996
0.625000000	0.666670024	0.172812998
0.625630021	0.666559994	0.321020991
0.625000000	0.666670024	0.025953000
0.874759972	0.833498001	0.246926993
0.875000000	0.833329976	0.099382997
0.866334975	0.833454013	0.401594996
0.446090996	0.339560986	0.507902980
0.614221990	0.273622006	0.527849972
0.593765020	0.447842985	0.516580999
0.560150027	0.349222004	0.501896024
0.599309981	0.331811011	0.442543000

O\*

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B	As	O
36	36	1

Direct

0.000000000	0.000000000	0.099382997
0.970836997	0.999809027	0.376978993
0.250000000	0.166669995	0.025953000
0.254761010	0.166574001	0.321226001
0.250000000	0.166669995	0.172812998
0.999956012	0.000356000	0.246450007
0.500000000	0.000000000	0.099382997
0.468109995	0.001450000	0.377777994
0.750000000	0.166669995	0.025953000
0.748412013	0.168026999	0.321456999
0.750000000	0.166669995	0.172812998
0.500557005	0.000155000	0.246108994
0.000000000	0.333330005	0.099382997
0.970929027	0.332987010	0.377530992
0.250000000	0.500000000	0.025953000
0.254639000	0.500558972	0.321485996
0.250000000	0.500000000	0.172812998
0.000948000	0.333487988	0.246947005
0.500000000	0.333330005	0.099382997
0.520312011	0.343865007	0.402368009
0.750000000	0.500000000	0.025953000
0.748438001	0.499339014	0.321375012
0.750000000	0.500000000	0.172812998
0.500253022	0.333521008	0.246720001
0.000000000	0.666670024	0.099382997
0.970647991	0.666980028	0.376875997
0.250000000	0.833329976	0.025953000
0.252205998	0.833487988	0.320670992
0.250000000	0.833329976	0.172812998
0.000086000	0.666667998	0.246463001



0.500000000	0.666670024	0.099382997
0.467772990	0.667346001	0.378246009
0.750000000	0.833329976	0.025953000
0.749162972	0.833361983	0.320802003
0.750000000	0.833329976	0.172812998
0.500481009	0.666621983	0.246126994
0.125000000	0.000000000	0.172812998
0.128828004	0.000024000	0.320149988
0.125000000	0.000000000	0.025953000
0.376419008	0.166614994	0.246467993
0.375000000	0.166669995	0.099382997
0.362982988	0.162881002	0.401511014
0.625000000	0.000000000	0.172812998
0.626264989	0.000149000	0.320342988
0.625000000	0.000000000	0.025953000
0.875054002	0.167218000	0.247031003
0.875000000	0.166669995	0.099382997
0.865296006	0.166455001	0.401358992
0.125000000	0.333330005	0.172812998
0.130230993	0.333494008	0.320948988
0.125000000	0.333330005	0.025953000
0.376138985	0.500156999	0.246668994
0.375000000	0.500000000	0.099382997
0.361032993	0.505518019	0.402393997
0.625000000	0.333330005	0.172812998
0.622793972	0.333317995	0.319920003
0.625000000	0.333330005	0.025953000
0.875088990	0.499740005	0.246999994
0.875000000	0.500000000	0.099382997
0.865543008	0.499862999	0.401077986

0.125000000	0.666670024	0.172812998
0.128906995	0.666643023	0.320120007
0.125000000	0.666670024	0.025953000
0.376147985	0.833387971	0.246588007
0.375000000	0.833329976	0.099382997
0.360433996	0.834252000	0.403034002
0.625000000	0.666670024	0.172812998
0.625712991	0.666823983	0.320558995
0.625000000	0.666670024	0.025953000
0.875379026	0.833411992	0.246895000
0.875000000	0.833329976	0.099382997
0.865634978	0.833384991	0.401437998
0.602042973	0.336542994	0.446258008

OH\*

9.5539999008	0.0000000000	0.0000000000
0.0000000000	10.1335000992	0.0000000000
0.0000000000	0.0000000000	23.0000000000

B As H O

36 36 1 1

Direct

0.000000000	0.000000000	0.099382997
0.971750975	0.000189000	0.377140999
0.250000000	0.166669995	0.025953000
0.253814995	0.166510999	0.321433008
0.250000000	0.166669995	0.172812998
0.000094000	0.000445000	0.246390000
0.500000000	0.000000000	0.099382997
0.467101008	0.000759000	0.378560007
0.750000000	0.166669995	0.025953000
0.748485982	0.168769002	0.321410000

0.750000000	0.166669995	0.172812998
0.500953972	0.000437000	0.246498004
0.000000000	0.333330005	0.099382997
0.971957028	0.332785010	0.377184987
0.250000000	0.500000000	0.025953000
0.253037006	0.500675023	0.320924014
0.250000000	0.500000000	0.172812998
0.000543000	0.333618999	0.246526003
0.500000000	0.333330005	0.099382997
0.501357019	0.329852015	0.398754001
0.750000000	0.500000000	0.025953000
0.747988999	0.498730004	0.320645005
0.750000000	0.500000000	0.172812998
0.500949979	0.333595008	0.246956006
0.000000000	0.666670024	0.099382997
0.971408010	0.667432010	0.377490014
0.250000000	0.833329976	0.025953000
0.250692993	0.833460987	0.320520997
0.250000000	0.833329976	0.172812998
0.999876022	0.666965008	0.246251002
0.500000000	0.666670024	0.099382997
0.466845006	0.667527974	0.377963006
0.750000000	0.833329976	0.025953000
0.749728024	0.833974004	0.321060985
0.750000000	0.833329976	0.172812998
0.500630975	0.666876972	0.246345997
0.125000000	0.000000000	0.172812998
0.128977999	0.000952000	0.319867015
0.125000000	0.000000000	0.025953000
0.376266986	0.167063996	0.246711001

0.375000000	0.166669995	0.099382997
0.363775998	0.166492000	0.401533991
0.625000000	0.000000000	0.172812998
0.626573026	0.001118000	0.321162999
0.625000000	0.000000000	0.025953000
0.874876976	0.167422995	0.247087002
0.875000000	0.166669995	0.099382997
0.866778016	0.166665003	0.401486993
0.125000000	0.333330005	0.172812998
0.130119994	0.333442986	0.320239991
0.125000000	0.333330005	0.025953000
0.376325011	0.500231028	0.246436998
0.375000000	0.500000000	0.099382997
0.365570009	0.500977993	0.399886012
0.625000000	0.333330005	0.172812998
0.621231019	0.333988994	0.321170986
0.625000000	0.333330005	0.025953000
0.875106990	0.500145018	0.246861994
0.875000000	0.500000000	0.099382997
0.867299020	0.500006020	0.400766999
0.125000000	0.666670024	0.172812998
0.128224999	0.666544020	0.319869012
0.125000000	0.666670024	0.025953000
0.376139998	0.833679974	0.246726006
0.375000000	0.833329976	0.099382997
0.362224996	0.834056973	0.402130991
0.625000000	0.666670024	0.172812998
0.626688004	0.667181015	0.320659995
0.625000000	0.666670024	0.025953000
0.875333011	0.833796978	0.246877998

0.875000000	0.833329976	0.099382997
0.866320014	0.833863020	0.401843995
0.652020991	0.399313986	0.452118009
0.586845994	0.325028002	0.448630005

H<sub>2</sub>O\*

9.5539999008	0.000000000	0.000000000
0.000000000	10.133500092	0.000000000
0.000000000	0.000000000	23.000000000

B	As	H	O
36	36	2	1

Direct

0.000000000	0.000000000	0.099382997
0.970685005	0.998594999	0.378526986
0.250000000	0.166669995	0.025953000
0.253459990	0.166427001	0.321985990
0.250000000	0.166669995	0.172812998
0.000510000	0.000178000	0.246441007
0.500000000	0.000000000	0.099382997
0.469040990	0.000694000	0.378592998
0.750000000	0.166669995	0.025953000
0.749031007	0.168119997	0.319501013
0.750000000	0.166669995	0.172812998
0.500212014	0.000049000	0.246400997
0.000000000	0.333330005	0.099382997
0.972348988	0.333723992	0.377804011
0.250000000	0.500000000	0.025953000
0.253291011	0.500602007	0.321891993
0.250000000	0.500000000	0.172812998
0.001014000	0.333415985	0.246489003
0.500000000	0.333330005	0.099382997

0.496769011	0.333537012	0.391719013
0.750000000	0.500000000	0.025953000
0.748969018	0.498843998	0.319453001
0.750000000	0.500000000	0.172812998
0.500015020	0.333460003	0.246197000
0.000000000	0.666670024	0.099382997
0.970808029	0.668706000	0.378515005
0.250000000	0.833329976	0.025953000
0.249556005	0.833519995	0.321006000
0.250000000	0.833329976	0.172812998
0.000480000	0.666697979	0.246414006
0.500000000	0.666670024	0.099382997
0.468901008	0.666336000	0.378564000
0.750000000	0.833329976	0.025953000
0.750047982	0.833459020	0.320787996
0.750000000	0.833329976	0.172812998
0.500065982	0.666844010	0.246391997
0.125000000	0.000000000	0.172812998
0.127734005	0.000964000	0.320739001
0.125000000	0.000000000	0.025953000
0.375562996	0.166693002	0.246949002
0.375000000	0.166669995	0.099382997
0.365758985	0.167355999	0.402485013
0.625000000	0.000000000	0.172812998
0.626960993	0.000329000	0.320865005
0.625000000	0.000000000	0.025953000
0.876188993	0.166795000	0.246603996
0.875000000	0.166669995	0.099382997
0.866671979	0.167297006	0.400595009
0.125000000	0.333330005	0.172812998

0.130128995	0.333516002	0.320656002
0.125000000	0.333330005	0.025953000
0.375528008	0.500205994	0.246913001
0.375000000	0.500000000	0.099382997
0.365671009	0.499605000	0.402379006
0.625000000	0.333330005	0.172812998
0.623097003	0.333438993	0.319348991
0.625000000	0.333330005	0.025953000
0.876222014	0.500055015	0.246601999
0.875000000	0.500000000	0.099382997
0.866685987	0.500153005	0.400566995
0.125000000	0.666670024	0.172812998
0.127712995	0.666119993	0.320686996
0.125000000	0.666670024	0.025953000
0.375220001	0.833467007	0.247001007
0.375000000	0.833329976	0.099382997
0.363656998	0.833545029	0.402213991
0.625000000	0.666670024	0.172812998
0.626811981	0.666656017	0.320809007
0.625000000	0.666670024	0.025953000
0.875787973	0.833432019	0.246996999
0.875000000	0.833329976	0.099382997
0.863937020	0.833563030	0.403061986
0.665925980	0.412169009	0.444521010
0.666779995	0.255856991	0.444317013
0.600233018	0.333683014	0.446455002

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